

1-Hexanol
111-27-3 | DTXSID8021931

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -61.5 °C

Global applicability domain: Inside

Local applicability domain index: 8.77e-01

Confidence level: 6.19e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Hexanol</div> <div>Measured: -44.6</div> <div>Predicted: -61.5</div>	<div>Image not found</div> <div>1-Heptanol</div> <div>Measured: -34.0</div> <div>Predicted: -47.4</div>	<div>Image not found</div> <div>Isopentyl alcohol</div> <div>Measured: -117</div> <div>Predicted: -96.2</div>
<div>Image not found</div> <div>1-Pentanol</div> <div>Measured: -78.9</div> <div>Predicted: -87.1</div>	<div>Image not found</div> <div>3,3-Dimethyl-1-butanol</div> <div>Measured: -60.0</div> <div>Predicted: -40.7</div>	